CONTENTS

Torsional vibrations in two-photon resonance spectroscopy of toluene derivatives
J.G. Philis (Ioannina, Greece) and L. Goodman (New Brunswick, NJ, U.S.A.) 1

Molecular structure of 1,1,1-trichloroethane
T. Iijima and R.-I. Wada (Tokyo, Japan) 7

The gas-phase molecular structures of monomeric and dimeric bis(dimethylamino)tin(II), $Sn(NMe_2)_2$. An electron diffraction study
B. Beagley and N.G. Scott (Manchester, Gt. Britain) and D. Schmidling (New York, NY, U.S.A.) 15

Instant ligands. Part 5. The molecular structures of $(PF_2)OCH_2C{=}CCH_2O(PF_2)$ in the gas phase and $PF_2OCH_2CH_2CN$ in gaseous and crystalline phases
A.J. Blake, M.J. Davis and D.W.H. Rankin (Edinburgh, Gt. Britain) 25

Determination of the gas-phase molecular structure of bis(trimethylsilyl)sulphide by electron diffraction and molecular mechanics calculations
D.G. Anderson, G.A. Forsyth and D.W.H. Rankin (Edinburgh, Gt. Britain) 45

Electron diffraction analysis of XY_2 and XY_3 molecules with large amplitude motion. Part I. Dynamical model and molecular scattering function
V.P. Spiridonov (Moscow, U.S.S.R.), A.G. Gershikov (Donetsk, U.S.S.R.) and V.S. Lyutsarev (Moscow, U.S.S.R.) 57

Electron diffraction analysis of XY_2 and XY_3 molecules with large amplitude motion. Part II. Survey of experimental studies
V.P. Spiridonov (Moscow, U.S.S.R.), A.G. Gershikov (Donetsk, U.S.S.R.) and V.S. Lyutsarev (Moscow, U.S.S.R.) 79

Conformational structures, energies, rotational barrier heights and torsional force constants in the acid halides $XH_2C{-}CYO$ and $X_2HC{-}CYO$ (Y = F, Cl, Br and X = Cl, Br)
A. Lund and R. Stølevik (Dragvoll, Norway) 95

Torsional potentials in halogen derivatives of 2-methylpropanal obtained by molecular mechanics calculations
L.G. Faksness and R. Stølevik (Dragvoll, Norway) 103

The influence of steric effects on proton-transfer equilibrium in intramolecular hydrogen bonds
M. Rospenk (Wrocław, Poland) 109

Rotational isomerism in 2-methyl-1,2-dinitropropane
Y.L. Lam, B.G. Tan and H.H. Huang (Singapore, Singapore) 115

Adsorption and reaction of *trans*-cinnamonitrile on a silver surface investigated by Raman spectroscopy
H.A. Chun, M.S. Kim and K. Kim (Seoul, Korea) 127

Vibrational spectra and conformation of diallyl disulphide in the liquid state
H. Suzuki, K. Fukushi, S.-I. Ikawa and S. Konaka (Sapporo, Japan) 141

The Morse-like potential model accounting for a stretch–bend interaction in linear XYZ molecules
B.S. Butayev, V.S. Lyutsarev, A.S. Saakyan and V.P. Spiridonov (Moscow, U.S.S.R.) 149

Ab initio vibrational analysis of *trans*- and *gauche*-2,3-dimethylbuta-1,3-diene
C.W. Bock (Marcus Hook, PA, U.S.A.) and Y.N. Panchenko (Moscow, U.S.S.R.) 159

Molecular geometry and frequencies of vibration of the molecule Li_2CO_3
F. Ramondo and L. Bencivenni (Rome, Italy) 169

Hydrogen bonds with large proton polarizability in films of $(L\text{-his})_n$ and $(L\text{-lys})_n$ with a model molecule of the head group of phosphatidylserine: proton conduction in polar surfaces of biological membranes
K. Leberle and G. Zundel (Munich, F.R.G.) 175

Hydrogen bonding. Part 32. Strong hydrogen bonding as the driving force for the solubilization of phthalic acid by fluoride ion
K.M. Harmon, L.M. Pappalardo and P.K. Keefer (Rochester, MI, U.S.A.) 189
Vibrational levels connected with reaction coordinate in conformer interconversion processes: application of the phase integral method to torsional energy levels
T. Raaska, H. Kunttu, M. Räsänen, J. Luppi and P. Pajunen (Helsinki, Finland) 195
Which tautomeric form of 5-methylcytosine predominates in vacuum?
A. Leś and L. Adamowicz (Tucson, AZ, U.S.A.) 209
A dipole moment study of (*Z*)-α,β-diarylacrylonitriles
M.E. Amato and G. Scarlata (Catania, Italy), J. Curé and H. Lumbroso (Paris, France) 219
$[N–H\cdots N]^+$ and $[H–H\cdots N]^-$ intramolecular hydrogen bonds in the complex of 1,8-bis(dimethylamino)naphthalene with 1,8-bis(4-toluenesulphonamide)-2,4,5,7-tetranitronaphthalene
Z. Malarski and T. Lis (Wrocław, Poland), E. Grech and J. Nowicka-Scheibe (Szczecin, Poland) and K. Majewska (Katowice, Poland) 227
An answer to the SPIRO versus ANSA dilemma in cyclophosphazenes. Part XIV. The first MACRO-BINO and MEGA-BINO species from oxodiamines
F. Sournies, P. Castera, A. El Bakili and J.-F. Labarre (Toulouse, France) 239
An answer to the SPIRO versus ANSA dilemma in cyclophosphazenes. Part XV. The first MACRO-diBINO and MEGA-diBINO non-geminal species from oxodiamines
F. Sournies, P. Castera, J.-P. Faucher, M. Graffeuil and J.-F. Labarre (Toulouse, France) 245
Crystal and molecular structure of the first DIBINO non-geminal macrocyclic dicyclophosphazene $\{N_3P_3Cl_4[HN–(CH_2)_3–O–(CH_2)_2–O–(CH_2)_3–NH]\}_2$
R. Enjalbert, J. Galy, F. Sournies and J.-F. Labarre (Toulouse, France) 253
Crystal structure of bis(pyridine betaine) hydrochloride monohydrate
X.-M. Chen and T.C.W. Mak (Shatin, Hong Kong) 265
A novel 1 : 1 canal inclusion network formed by deoxycholic acid dimers (bislactones) with benzene molecules: an X-ray study
S. Stanković (Novi Sad, Yugoslavia), A. Kálmán and Gy. Argay (Budapest, Hungary), D. Miljković and K. Kuhajda (Novi Sad, Yugoslavia), I. Vicković and M. Bruwo (Zagreb, Yugoslavia) and O. Ori (Parma, Italy) 271
Electron spin resonance of gamma irradiated single crystals of acetylcholine iodide and bromide
F. Köksal, M. Birey, R. Tapramaz and F. Çelik (Samsun, Turkey) 283
The structure and mobility of L-alanine residues of tropomyosin in the solid state as studied by high resolution solid state ^{13}C NMR spectroscopy
S. Tuzi, S. Sakamaki and I. Ando (Tokyo, Japan) 289
^1H and ^{13}C NMR study of substituted 3-OH pyridines
D.G. De Kowalewski and C. De Los Santos (Buenos Aires, Argentina) 299
^{13}C NMR spectra and enol–enol tautomerism in crystalline keto–enols
A.I. Kol'tsov and A.A. Elkin (Leningrad, U.S.S.R.) and D.Kh. Zheglova (Sofia, Bulgaria) 309

Short communication
Molecular structure of gaseous xanthene by electron diffraction
K. Iijima, T. Misu and S. Onuma (Shizuoka, Japan) 315

Book reviews 319

Author index 325

Subject index 327